Package 'parallelpam'

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Type Package Title Parallel Partitioning-Around-Medoids (PAM) for Big Sets of Data Version 1.0.1 Author Juan Domingo [aut, cre] (<https://orcid.org/0000-0003-4728-6256>), Guillermo Ayala [ctb] (<https://orcid.org/0000-0002-6231-2865>), Spanish Ministry of Science and Innovation, MCIN/AEI <doi:10.13039/501100011033> [fnd] Maintainer Juan Domingo <Juan.Domingo@uv.es> Description Application of the Partitioning-Around-Medoids (PAM) clustering algorithm described in Schubert, E. and Rousseeuw, P.J.: ``Fast and eager k-medoids clustering: O(k) runtime improvement of the PAM, CLARA, and CLARANS algorithms." Information Systems, vol. 101, p. 101804, (2021). <doi:10.1016/j.is.2021.101804>. It uses a binary format for storing and retrieval of matrices developed for the 'jmatrix' package but the functionality of 'jmatrix' is included here, so you do not need to install it. Also, it is used by package 'scellpam', so if you have installed it, you do not need to install this package. PAM can be applied to sets of data whose dissimilarity matrix can be very big. It has been tested with up to 100.000 points. It does this with the help of the code developed for other package, 'jmatrix', which allows the matrix not to be loaded in 'R' memory (which would force it to be of double type) but it gets from disk, which allows using float (or even smaller data types). Moreover, the dissimilarity matrix is calculated in parallel if the computer has several cores so it can open many threads. The initial part of the PAM algorithm can be done with the BUILD or LAB algorithms; the BUILD algorithm has been implemented in parallel. The optimization phase implements the FastPAM1 algorithm, also in parallel. Finally, calculation of silhouette is available and also implemented in parallel. **License** GPL (≥ 2) **Imports** Rcpp (>= 1.0.8), memuse (>= 4.2.1)

LinkingTo Rcpp

SystemRequirements C++14

ApplyPAM

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ApplyPAM

Description

A function to implement the Partitioning-around-medoids algorithm described in Schubert, E. and Rousseeuw, P.J.: "Fast and eager k-medoids clustering: O(k) runtime improvement of the PAM, CLARA, and CLARANS algorithms." Information Systems, vol. 101, p. 101804, 2021. doi: https://doi.org/10.1016/j.is.2021.101804 Notice that the actual values of the vectors (instances) are not needed. To recover them, look at the data matrix used to generate the distance matrix.

The number of instances, N, is not passed since dissimilarity matrix is NxN and therefore its size indicates the N value.

Usage

```
ApplyPAM(
   dissim_file,
   k,
   init_method = "BUILD",
   initial_med = NULL,
   max_iter = 1000L,
   nthreads = 0L
)
```

Arguments

dissim_file	A string with the name of the binary file that contains the symmetric matrix of dissimilarities. Such matrix should have been generated by CalcAndWrite-DissimilarityMatrix and it is a matrix of type 'disttype' (in this type defined as float).
k	A possitive integer (the desired number of medoids).
init_method	One of the strings 'PREV', 'BUILD' or 'LAB'. See meaning of initialization algorithms BUILD and LAB in the original paper. 'PREV' should be used exclusively to start the second part of the algorithm (optimization) from a initial set of medoids generated by a former call. Default: BUILD.
initial_med	A vector with initial medoids to start optimization. It is to be used only by the 'PREV' method and it will have been obtained as the first element (L\$med) of the two-element list returned by a previous call to this function used in just-initialize mode (max_iter=0). Default: empty vector.
max_iter	The maximum number of allowed iterations. 0 means stop immediately after finding initial medoids. Default: 1000
nthreads	For the BUILD initialization algorithm (the only part currently implemented in parallel), the number of used threads. -1 means don't use threads (serial implementation). 0 means let the program choose according to the number of cores and of points.

Any other number forces this number of threads. Choosing more than the number of available cores is allowed, but discouraged. Default: 0

Details

With respect to the returned value, L\$med has as many components as requested medoids and L\$clasif has as many components as instances.

Medoids are expressed in L\$med by its number in the array of points (row in the dissimilarity matrix) starting at 1 (R convention).

L\$clasif contains the number of the medoid (i.e.: the cluster) to which each instance has been assigned, according to their order in

L\$med (also from 1).

This means that if L\$clasif[p] is m, the point p belongs to the class grouped around medoid L\$med[m].

Moreover, if the dissimilarity matrix contains as metadata the point names, the returned are Rnamed vector with such names.

Value

L["med","clasif"] A list of two numeric vectors. See section Details for more information

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
{
 p<-20*runif(500)</pre>
 Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)</pre>
 for (k in (1:10))
 {
 M[10*(i-1)+k,]=p+Rf[k,]
 }
}
JWriteBin(M, "pamtest.bin", dtype="float", dmtype="full")
CalcAndWriteDissimilarityMatrix("pamtest.bin","pamDL2.bin",distype="L2",restype="float",nthreads=0)
L <- ApplyPAM("pamDL2.bin",10,init_method="BUILD")</pre>
# Final value of sum of distances to closest medoid
GetTD(L,"pamDL2.bin")
# Medoids:
L$med
# Medoid in which each individual has been classified
n<-names(L$med)</pre>
n[L$clasif]
file.remove("pamtest.bin")
file.remove("pamDL2.bin")
```

CalcAndWriteDissimilarityMatrix CalcAndWriteDissimilarityMatrix

Description

Writes a binary symmetric matrix with the dissimilarities between ROWS of the data stored in a binary matrix in the scellpam package format.

Notice that, differently from the common practice in single cell, the rows represent cells. This is for efficiency reasons and it is transparent to the user, as long as he/she has generated the binary matrix (with CsvToBinMat, dgCMatToBinMat or SceToBinMat) using the option transpose=TRUE.

The input matrix of vectors can be a full or a sparse matrix. Output matrix type can be float or double type (but look at the comments in 'Details').

Usage

```
CalcAndWriteDissimilarityMatrix(
    ifname,
    ofname,
    distype = "L2",
    restype = "float",
    comment = "",
    nthreads = 0L
)
```

Arguments

A string with the name of the file containing the counts as a binary matrix, as written by CsvToBinMat, dgCMatToBinMat or SceToBinMat
A string with the name of the binary output file to contain the symmetric dis- similarity matrix.
The dissimilarity to be calculated. It must be one of these strings: 'L1', 'L2' or 'Pearson'. Default: 'L2'.
The data type of the result. It can be one of the strings 'float' or 'double'. Default: float (and don't change it unless you REALLY need to).
Comment to be added to the dissimilary matrix. Default: "" (no comment)
 Number of threads to be used for the parallel calculations with this meaning: -1: don't use threads. 0: let the function choose according to the number of individuals (cells) and to the number of available cores. Any possitive number > 1: use that number of threads. You can use even more than cores, but this is discouraged and raises a warning. Default: 0.

Details

The parameter restype forces the output to be a matrix of either floats or doubles. Precision of float if normally good enough; but if you need double precision (may be because you expect your results to be in a large range, two to three orders of magnitude), change it.

Nevertheless, notice that this at the expense of double memory usage, which is QUADRATIC with the number of individuals (rows) in your input matrix.

Value

No return value, called for side effects (creates a file)

Examples

```
Rf <- matrix(runif(50000),nrow=100)</pre>
JWriteBin(Rf, "Rfullfloat.bin", dtype="float", dmtype="full",
          comment="Full matrix of floats, 100 rows, 500 columns")
JMatInfo("Rfullfloat.bin")
CalcAndWriteDissimilarityMatrix("Rfullfloat.bin","RfullfloatDis.bin",distype="L2",
                       restype="float",comment="L2 distance matrix from full",nthreads=0)
JMatInfo("RfullfloatDis.bin")
JWriteBin(Rf, "Rsparsefloat.bin", dtype="float", dmtype="sparse",
                        comment="Sparse matrix of floats, 100 rows, 500 columns")
JMatInfo("Rsparsefloat.bin")
CalcAndWriteDissimilarityMatrix("Rsparsefloat.bin","RsparsefloatDis.bin",distype="L2",
                     restype="float",comment="L2 distance matrix from sparse",nthreads=0)
JMatInfo("RsparsefloatDis.bin")
Dfu<-GetJManyRows("RfullfloatDis.bin",c(1:nrow(Rf)))</pre>
Dsp<-GetJManyRows("RsparsefloatDis.bin",c(1:nrow(Rf)))</pre>
max(Dfu-Dsp)
file.remove("Rfullfloat.bin")
file.remove("Rsparsefloat.bin")
file.remove("RfullfloatDis.bin")
file.remove("RsparsefloatDis.bin")
```

CalculateSilhouette CalculateSilhouette

Description

Calculates the silhouette of each point of those classified by a clustering algorithm.

Usage

```
CalculateSilhouette(cl, fdist, nthreads = 0L)
```

Arguments

cl	The array of classification with the number of the class to which each point be- longs to. This number must be in 1number_of_classes. This function takes something like the L\$clasif array which is the second ele- ment of the list returned by ApplyPAM
fdist	The binary file containing the symmetric matrix with the dissimilarities between points (usually, generated by a call to CalcAndWriteDissimilarityMatrix)
nthreads	The number of used threads. -1 means don't use threads (serial implementation). 0 means let the program choose according to the number of cores and of points. Any other number forces this number of threads. Choosing more than the number of available cores is allowed, but discouraged. Default: 0

Value

sil Numeric vector with the values of the silhouette for each point, in the same order in which points are in cl.

If cl is a named vector sill will be a named vector, too, with the same names.

Examples

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
{
 p<-20*runif(500)</pre>
 Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)</pre>
 for (k in (1:10))
 {
 M[10*(i-1)+k,]=p+Rf[k,]
 }
}
JWriteBin(M, "pamtest.bin", dtype="float", dmtype="full")
CalcAndWriteDissimilarityMatrix("pamtest.bin","pamDL2.bin",distype="L2",restype="float",nthreads=0)
L <- ApplyPAM("pamDL2.bin",10,init_method="BUILD")</pre>
sil <- CalculateSilhouette(L$clasif,"pamDL2.bin")</pre>
# Histogram of the silhouette. In this synthetic problem, almost 1 for all points
hist(sil)
file.remove("pamtest.bin")
file.remove("pamDL2.bin")
```

ClassifAsDataFrame ClassifAsDataFrame

Description

Returns the results of the classification returned by ApplyPAM as a R dataframe

Usage

```
ClassifAsDataFrame(L, fdist)
```

Arguments

L	The list returned by ApplyPAM with fields L\$med and
	L\$clasif with the numbers of the medoids and the classification of each point
fdist	The binary file containing the symmetric matrix with the dissimilarities between points (usually, generated by a call to CalcAndWriteDissimilarityMatrix or to
	CalcAndWriteDissimilarityMatrixDouble)

Details

The dataframe has three columns: PointName (name of each point), NNPointName (name of the point which is the center of the cluster to which PointName belongs to) and NNDistance (distance between the points PointName and NNPointName). Medoids are identified by the fact that PointName and NNPointName are equal, or equivalently, NNDistance is 0.

Value

Df Dataframe with columns PointName, NNPointName and NNDistance. See Details for description.

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
{
 p<-20*runif(500)</pre>
 Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)</pre>
 for (k in (1:10))
 {
 M[10*(i-1)+k,]=p+Rf[k,]
 }
}
JWriteBin(M, "pamtest.bin", dtype="float", dmtype="full")
CalcAndWriteDissimilarityMatrix("pamtest.bin","pamDL2.bin",distype="L2",restype="float",nthreads=0)
L <- ApplyPAM("pamDL2.bin",10,init_method="BUILD")</pre>
df <- ClassifAsDataFrame(L,"pamDL2.bin")</pre>
df
# Identification of medoids:
which(df[,3]==0)
# Verification they are the same as in L (in different order)
L$med
```

```
file.remove("pamtest.bin")
file.remove("pamDL2.bin")
```

FilterBySilhouetteQuantile FilterBySilhouetteQuantile

Description

Takes a silhouette, as returned by CalculateSilhouette, the list of medoids and class assignments, as returned by ApplyPam, a quantile and the matrices of counts and dissimilarities and constructs the corresponding matrices clearing off the points whose silhoutte is below the lower quantile, except if they are medoids.

Usage

```
FilterBySilhouetteQuantile(
    s,
    L,
    fallcounts,
    ffilcounts,
    falldissim,
    ffildissim,
    q = 0.2,
    addcom = TRUE
)
```

Arguments

S	A numeric vector with the sihouette coefficient of each point in a classification, as returned by CalculateSilhouette.
L	A list of two numeric vectors, L\$med and L\$clasif, obtained normally as the object returned by ApplyPAM.
fallcounts	A string with the name of the binary file containing the matrix of individuals. It can be either a full or a sparse matrix.
ffilcounts	A string with the name of the binary file that will contain the selected individu- als. It will have the same character (full/sparse) and type of the complete file.
falldissim	A string with the name of the binary file containing the dissimilarity matrix of the complete set of individuals. It must be a symmetric matrix of floats.
ffildissim	A string with the name of the binary file that will contain the dissimilarity matrix for the remaining individuals. It will be a symmetric matrix of floats.
q	Quantile to filter. All points whose silhouette is below this quantile will be filtered out. Default: 0.2

addcom Boolean to indicate if a comment must be appended to the current comment of counts and dissimilarity matrices to indicate that they are the result of a filtering process. This comment is automatically generated and contains the value of quantile q. Succesive applications add comments at the end of those already present. Default: TRUE

Details

The renumbering of indices in the returned cluster may seem confusing at first but it was the way of fitting this with the rest of the package. Anyway, notice that if the numeric vectors in the input parameter L were named vectors, the point names are appropriately kept in the result so point identity is preserved. Moreover, if the counts and dissimilarity input matrices had row and/or column names, they are preserved in the filtered matrices, too.

Value

Lr["med","clasif"] A list of two numeric vectors.

Lr\$med is a modification of the correponding first element of the passed L parameter.

Lr\$clasif has as many components as remaining instances.

Since points will have been removed, medoid numbering is modified. Therefore, Lr\$med has the NEW index of each medoid in the filtered set.

Lr\$clasif contains the number of the medoid (i.e.: the cluster) to which each instance has been assigned, and therefore does not change.

All indexes start at 1 (R convention). Please, see Details section

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
{
 p<-20*runif(500)</pre>
 Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)</pre>
 for (k in (1:10))
 {
  M[10*(i-1)+k,]=p+Rf[k,]
 }
}
JWriteBin(M, "pamtest.bin", dtype="float", dmtype="full")
CalcAndWriteDissimilarityMatrix("pamtest.bin","pamDL2.bin",distype="L2",restype="float",nthreads=0)
L <- ApplyPAM("pamDL2.bin",10,init_method="BUILD")</pre>
# Which are the medoids
1 $med
sil <- CalculateSilhouette(L$clasif,"pamDL2.bin")</pre>
Lf<-FilterBySilhouetteQuantile(sil,L,"pamtest.bin","pamtestfilt.bin","pamDL2.bin","pamDL2filt.bin",
                                 q=0.4, addcom=TRUE)
# The new medoids are the same points but renumbered, since the L$clasif array has less points
Lf$med
```

file.remove("pamtest.bin")
file.remove("pamDL2.bin")
file.remove("pamtestfilt.bin")
file.remove("pamDL2filt.bin")

FilterBySilhouetteThreshold

FilterBySilhouetteThreshold

Description

Takes a silhouette, as returned by CalculateSilhouette, the list of medoids and class assignments, as returned by ApplyPam, a threshold and the matrices of counts and dissimilarities and constructs the corresponding matrices clearing off the points whose silhoutte is below the threshold, except if they are medoids.

Usage

```
FilterBySilhouetteThreshold(
    s,
    L,
    fallcounts,
    ffilcounts,
    falldissim,
    ffildissim,
    thres = 0,
    addcom = TRUE
)
```

Arguments

S	A numeric vector with the sihouette coefficient of each point in a classification, as returned by CalculateSilhouette.
L	A list of two numeric vectors, L\$med and L\$clasif, obtained normally as the object returned by ApplyPAM.
fallcounts	A string with the name of the binary file containing the matrix of counts per individuals. It can be either a full or a sparse matrix.
ffilcounts	A string with the name of the binary file that will contain the selected individu- als. It will have the same character (full/sparse) and type of the complete file.
falldissim	A string with the name of the binary file containing the dissimilarity matrix of the complete set of individuals. It must be a symmetric matrix of floats.
ffildissim	A string with the name of the binary file that will contain the dissimilarity matrix for the remaining individuals. It will be a symmetric matrix of floats.
thres	Threshold to filter. All points whose silhouette is below this threshold will be filtered out. Default: 0.0 (remember that silhouette is in [-11])

addcom Boolean to indicate if a comment must be appended to the current comment of counts and dissimilarity matrices to indicate that they are the result of a filtering process. This comment is automatically generated and contains the value of threshold t. Succesive applications add comments at the end of those already present. Default: TRUE

Details

The renumbering of indices in the returned cluster may seem confusing at first but it was the way of fitting this with the rest of the package. Anyway, notice that if the numeric vectors in the input parameter L were named vectors, the point names are appropriately kept in the result so point identity is preserved. Moreover, if the individuals and dissimilarity input matrices had row and/or column names, they are preserved in the filtered matrices, too.

Value

Lr["med", "clasif"] A list of two numeric vectors.

Lr\$med is a modification of the correponding first element of the passed L parameter.

Lr\$clasif has as many components as remaining instances.

Since points will have been removed, medoid numbering is modified. Therefore, Lr\$med has the NEW index of each medoid in the filtered set.

Lr\$clasif contains the number of the medoid (i.e.: the cluster) to which each instance has been assigned, and therefore does not change.

All indexes start at 1 (R convention). Please, see Details section

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
{
 p<-20*runif(500)</pre>
 Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)</pre>
 for (k in (1:10))
 {
  M[10*(i-1)+k,]=p+Rf[k,]
 }
}
JWriteBin(M, "pamtest.bin", dtype="float", dmtype="full")
CalcAndWriteDissimilarityMatrix("pamtest.bin","pamDL2.bin",distype="L2",restype="float",nthreads=0)
L <- ApplyPAM("pamDL2.bin",10,init_method="BUILD")</pre>
# Which are the medoids
1 $med
sil <- CalculateSilhouette(L$clasif,"pamDL2.bin")</pre>
Lf<-FilterBySilhouetteQuantile(sil,L,"pamtest.bin","pamtestfilt.bin","pamDL2.bin","pamDL2filt.bin",
                                  q=0.4, addcom=TRUE)
# The new medoids are the same points but renumbered, since the L$clasif array has less points
Lf$med
```

GetJCol

```
file.remove("pamtest.bin")
file.remove("pamDL2.bin")
file.remove("pamtestfilt.bin")
file.remove("pamDL2filt.bin")
```

GetJCol

GetJCol

Description

Returns (as a R numeric vector) the requested column number from the matrix contained in a jmatrix binary file

Usage

GetJCol(fname, ncol)

Arguments

fname	String with the file name that contains the binary data.
ncol	The number of the column to be returned, in R-numbering (from 1)

Value

A numeric vector with the values of elements in the requested column

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A", "B", "C", "D", "E", "F")
colnames(Rf) <- c("a", "b", "c", "d", "e", "f", "g", "h")
JWriteBin(Rf, "Rfullfloat.bin", dtype="float", dmtype="full", comment="Full matrix of floats")
Rf[,3]
vf<-GetJCol("Rfullfloat.bin", 3)
vf
file.remove("Rfullfloat.bin")</pre>
```

GetJColByName

Description

Returns (as a R numeric vector) the requested named column from the matrix contained in a jmatrix binary file

Usage

GetJColByName(fname, colname)

Arguments

fname	String with the file name that contains the binary data.
colname	The name of the column to be returned. If the matrix has no column names, or
	the name is not found, an empty vector is returned

Value

A numeric vector with the values of elements in the requested column

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A", "B", "C", "D", "E", "F")
colnames(Rf) <- c("a", "b", "c", "d", "e", "f", "g", "h")
JWriteBin(Rf, "Rfullfloat.bin", dtype="float", dmtype="full", comment="Full matrix of floats")
Rf[,"c"]
vf<-GetJColByName("Rfullfloat.bin", "c")
vf
file.remove("Rfullfloat.bin")</pre>
```

GetJColNames GetJColNames

Description

Returns a R StringVector with the column names of a matrix stored in the binary format of package jmatrix, if it has them stored.

Usage

GetJColNames(fname)

GetJManyCols

Arguments

fname

String with the file name that contains the binary data.

Value

A R StringVector with the column names, or the empty vector if the binaryfile has no row column names as metadata.

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
JWriteBin(Rf,"Rfullfloat.bin",dtype="float",dmtype="full",comment="Full matrix of floats")
cn<-GetJColNames("Rfullfloat.bin")
cn
file.remove("Rfullfloat.bin")</pre>
```

GetJManyCols GetJManyCols

Description

Returns (as a R numeric matrix) the columns with the requested column numbers from the matrix contained in a jmatrix binary file

Usage

```
GetJManyCols(fname, extcols)
```

Arguments

fname	String with the file name that contains the binary data.
extcols	A numeric vector with the indexes of the columns to be extracted, in R-numbering
	(from 1)

Value

A numeric matrix with the values of elements in the requested columns

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
JWriteBin(Rf,"Rfullfloat.bin",dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[,c(1,4)]
vc<-GetJManyCols("Rfullfloat.bin",c(1,4))
vc
file.remove("Rfullfloat.bin")</pre>
```

GetJManyColsByNames GetJManyColsByNames

Description

Returns (as a R numeric matrix) the columns with the requested column names from the matrix contained in a jmatrix binary file

Usage

GetJManyColsByNames(fname, extcolnames)

Arguments

fname	String with the file name that contains the binary data.
extcolnames	A numeric vector with the names of the columns to be extracted. If the binary file has no column names, or _any_ of the column names is not present, an empty matrix is returned.

Value

A numeric matrix with the values of elements in the requested columns

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A", "B", "C", "D", "E", "F")
colnames(Rf) <- c("a", "b", "c", "d", "e", "f", "g", "h")
JWriteBin(Rf, "Rfullfloat.bin", dtype="float", dmtype="full", comment="Full matrix of floats")
Rf[,c(1,4)]
vf<-GetJManyColsByNames("Rfullfloat.bin", c("a", "d"))
vf
file.remove("Rfullfloat.bin")</pre>
```

GetJManyRows GetJManyRows

Description

Returns (as a R numeric matrix) the rows with the requested row numbers from the matrix contained in a jmatrix binary file

Usage

GetJManyRows(fname, extrows)

Arguments

fname	String with the file name that contains the binary data.
extrows	A numeric vector with the indexes of the rows to be extracted, in R-numbering (from 1)

Value

A numeric matrix with the values of elements in the requested rows

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
JWriteBin(Rf,"Rfullfloat.bin",dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[c(1,4),]
vc<-GetJManyRows("Rfullfloat.bin",c(1,4))
vc
file.remove("Rfullfloat.bin")</pre>
```

GetJManyRowsByNames GetJManyRowsByNames

Description

Returns (as a R numeric matrix) the rows with the requested row names from the matrix contained in a jmatrix binary file

Usage

GetJManyRowsByNames(fname, extrownames)

Arguments

fname	String with the file name that contains the binary data.
extrownames	A numeric vector with the names of the rows to be extracted. If the binary file has no row names, or _any_ of the row names is not present, an empty matrix is returned.

Value

A numeric matrix with the values of elements in the requested rows

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
JWriteBin(Rf,"Rfullfloat.bin",dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[c("A","C"),]
vf<-GetJManyRowsByNames("Rfullfloat.bin",c("A","C"))
vf
file.remove("Rfullfloat.bin")</pre>
```

GetJNames

GetJNames

Description

Returns a R list of two elements, rownames and colnames, each of them being a R StringVector with the corresponding names

Usage

GetJNames(fname)

Arguments

fname

String with the file name that contains the binary data.

Value

N["rownames", "colnames"]: A list with two elements named rownames and colnames which are R StringVectors. If the binary file has no row or column names as metadata BOTH will be returned as empty vectors, even if one of them exists. If you want to extract only one, use either GetBinRowNames or GetBinColNames, as appropriate.

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A", "B", "C", "D", "E", "F")
colnames(Rf) <- c("a", "b", "c", "d", "e", "f", "g", "h")
JWriteBin(Rf, "Rfullfloat.bin", dtype="float", dmtype="full", comment="Full matrix of floats")
N<-GetJNames("Rfullfloat.bin")
N["rownames"]
N["colnames"]
file.remove("Rfullfloat.bin")</pre>
```

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GetJRow

GetJRow

Description

Returns (as a R numeric vector) the requested row number from the matrix contained in a jmatrix binary file

Usage

GetJRow(fname, nrow)

Arguments

fname	String with the file name that contains the binary data.
nrow	The number of the row to be returned, in R-numbering (from 1)

Value

A numeric vector with the values of elements in the requested row

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
JWriteBin(Rf,"Rfullfloat.bin",dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[3,]
vf<-GetJRow("Rfullfloat.bin",3)
vf
file.remove("Rfullfloat.bin")</pre>
```

GetJRowByName GetJRowByName

Description

Returns (as a R numeric vector) the requested named row from the matrix contained in a jmatrix binary file

Usage

GetJRowByName(fname, rowname)

Arguments

fname	String with the file name that contains the binary data.
rowname	The name of the row to be returned. If the matrix has no row names, or the name
	is not found, an empty vector is returned

Value

A numeric vector with the values of elements in the requested row

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A", "B", "C", "D", "E", "F")
colnames(Rf) <- c("a", "b", "c", "d", "e", "f", "g", "h")
JWriteBin(Rf, "Rfullfloat.bin", dtype="float", dmtype="full", comment="Full matrix of floats")
Rf["C",]
vf<-GetJRowByName("Rfullfloat.bin", "C")
vf
file.remove("Rfullfloat.bin")</pre>
```

```
GetJRowNames
```

GetJRowNames

Description

Returns a R StringVector with the row names of a matrix stored in the binary format of package jmatrix, if it has them stored.

Usage

GetJRowNames(fname)

Arguments

fname String with the file name that contains the binary data.

Value

A R StringVector with the row names, or the empty vector if the binary file has no row names as metadata.

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A", "B", "C", "D", "E", "F")
colnames(Rf) <- c("a", "b", "c", "d", "e", "f", "g", "h")
JWriteBin(Rf, "Rfullfloat.bin", dtype="float", dmtype="full", comment="Full matrix of floats")
rn<-GetJRowNames("Rfullfloat.bin")
rn
file.remove("Rfullfloat.bin")</pre>
```

GetSubdiag

Description

Takes a symmetric matrix and returns a vector with all its elements under the main diagonal (without those at the diagonal itself) Done as an instrumental function to check the PAM in package cluster. To be removed in final version of the package.

Usage

GetSubdiag(fname)

Arguments

fname

The name of the file with the dissimilarity matrix in jmatrix binary format.

Value

The vector with the values under the main diagonal, sorted by columns (i.e.: m(2,1) ... m(n,1), m(3,2)...m(n,2),..., m(n-1,n))

Examples

```
Rns <- matrix(runif(49),nrow=7)
Rsym <- 0.5*(Rns+t(Rns))
rownames(Rsym) <- c("A", "B", "C", "D", "E", "F", "G")
colnames(Rsym) <- c("a", "b", "c", "d", "e", "f", "g")
JWriteBin(Rsym, "Rsymfloat.bin", dtype="float", dmtype="symmetric")
d<-GetSubdiag("Rsymfloat.bin")
Rsym
d
file.remove("Rsymfloat.bin")</pre>
```

GetTD

GetTD

Description

Function that takes a PAM classification (as returned by ApplyPAM) and the dissimilarity matrix and returns the value of the TD function (sum of dissimilarities between each point and its closest medoid, divided by the number of points). This function is mainly for debugging/internal use.

Usage

GetTD(L, dissim_file)

Arguments

L	A list of two numeric vectors, L["med", "clasif"], as returned by ApplyPAM (please, consult the help of ApplyPAM for details)
dissim_file	A string with the name of the binary file that contains the symmetric matrix of dissimilarities. Such matrix should have been generated by CalcAndWriteDis- similarityMatrix and it is a matrix of type 'disttype' (currently defined as float).

Value

TD The value of the TD function.

Examples

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
{
 p<-20*runif(500)</pre>
 Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)</pre>
 for (k in (1:10))
 {
 M[10*(i-1)+k,]=p+Rf[k,]
 }
}
JWriteBin(M, "pamtest.bin", dtype="float", dmtype="full")
CalcAndWriteDissimilarityMatrix("pamtest.bin","pamDL2.bin",distype="L2",restype="float",nthreads=0)
L <- ApplyPAM("pamDL2.bin",10,init_method="BUILD")</pre>
# Final value of sum of distances to closest medoid
GetTD(L,"pamDL2.bin")
```

JMatInfo

JMatInfo

Description

Shows in the screen or writes to a file information about a matrix stored in the binary format of package jmatrix

Usage

JMatInfo(fname, fres = "")

Arguments

fname	String with the file name that contains the binary data.
fres	String with the name of the file to write the information. Default: "" (information
	is written to the console)

JWriteBin

Value

No return value, called for its side effects (writes on screen or creates a file)

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
JWriteBin(Rf,"Rfullfloat.bin",dtype="float",dmtype="full",comment="Full matrix of floats")
JMatInfo("Rfullfloat.bin")
file.remove("Rfullfloat.bin")</pre>
```

|--|--|--|

Description

Writes a R matrix to a disk file as a binary matrix in the jmatrix format

Usage

```
JWriteBin(M, fname, dtype = "float", dmtype = "full", comment = "")
```

Arguments

М	The R matrix to be written
fname	The name of the file to write
dtype	The data type of the matrix to be written: one of the strings 'short', 'int', 'long', 'float' or 'double'. Default: 'float'
dmtype	The matrix type: one of the strings 'full', 'sparse' or 'symmetric'. Default: 'full'
comment	A optional string with the comment to be added as metadata. Default: "" (empty string, no added comment)

Details

Use this function cautiously. Differently to the functions to get one or more rows or columns from the binary file, which book only the memory strictly needed for the vector/matrix and do not load all the binary file in memory, this function books the full matrix in the requested data type and writes it later so with very big matrices you might run out of memory.

Type 'int' is really long int (8-bytes in most modern machines) so using 'int' or 'long' is equivalent. Type is coerced from double (the internal type of R matrices) to the requested type, which may provoke a loose of precision.

If M is a named-R matrix, row and column names are written as metadata, too.

Also, if you write as symmetric a matrix which is not such, only the lower-diagonal part will be written. The rest of the data will be lost. In this case, if the matrix has row and column names, only row names are written.

No return value, called for side effects (creates a file)

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
JWriteBin(Rf,"Rfullfloat.bin",dtype="float",dmtype="full",comment="Full matrix of floats")
file.remove("Rfullfloat.bin")</pre>
```

NumSilToClusterSil NumSilToClusterSil

Description

Takes a silhouette in the form of a NumericVector, as returned by CalculateSilhouette, and returns it as a numeric matrix appropriate to be plotted by the package 'cluster'

Usage

```
NumSilToClusterSil(cl, s)
```

Arguments

cl	The array of classification with the number of the class to which each point be- longs to. This number must be in 1number_of_classes. This function takes something like the L\$clasif array which is the second ele- ment of the list returned by ApplyPAM
S	The numeric value of the silhouette for each point, with points in the same order as they appear in cl. This is the vector returned by after a call to CalculateSilhouette with the same value of parameter cl.

Value

sp A silhouette in the format of the cluster package which is a NumericMatrix of as many rows as points and three columns: cluster, neighbor and sil_width.

Its structure and dimension names are as in package 'cluster', which allows to use it with the silhouette plotting functions of such package

This means you can do library(cluster) followed by plot(NumSilToClusterSil(cl,s)) to get a beatiful plot.

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ParallelpamSetDebug

Examples

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
{
 p<-20*runif(500)</pre>
 Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)</pre>
 for (k in (1:10))
 {
 M[10*(i-1)+k,]=p+Rf[k,]
 }
}
JWriteBin(M, "pamtest.bin", dtype="float", dmtype="full")
CalcAndWriteDissimilarityMatrix("pamtest.bin","pamDL2.bin",distype="L2",restype="float",nthreads=0)
L <- ApplyPAM("pamDL2.bin",10,init_method="BUILD")</pre>
sil <- CalculateSilhouette(L$clasif,"pamDL2.bin")</pre>
sp <- NumSilToClusterSil(L$clasif,sil)</pre>
# Here you can install and load package cluster and make plot(sp)
file.remove("pamtest.bin")
file.remove("pamDL2.bin")
```

ParallelpamSetDebug ParallelpamSetDebug

Description

Sets debugging in parallelpam package to ON (with TRUE) or OFF (with FALSE) for both parts of it.

On package load the default status is OFF.

Setting debugging of any part to ON shows a message. Setting to OFF does not show anything (since debugging is OFF...)

Usage

```
ParallelpamSetDebug(deb = TRUE, debjmat = FALSE)
```

Arguments

deb	boolean, TRUE to generate debug messages for the PAM algorithm and FALSE to turn them off. Default: true.
debjmat	boolean, TRUE to generate debug messages for the jmatrix part inside this pack- age and FALSE to turn them off. Default: false

Value

No return value, called for side effects (internal boolean flag changed)

Examples

ParallelpamSetDebug(TRUE,debjmat=TRUE)
ParallelpamSetDebug(TRUE,debjmat=FALSE)

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